

Electron-phonon interaction in the three-band model

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We study the half-breathing phonon in the three-band model of a high temperature superconductor, allowing for vibrations of atoms and resulting changes of hopping parameters. Two different approaches are compared. From the three-band model a t - J model with phonons can be derived, and phonon properties can be calculated. To make contact to density functional calculations, we also study the three-band model in the Hartree-Fock (HF) approximation. The paramagnetic HF solution, appropriate for the doped cuprates, has similarities to the local-density approximation (LDA). However, in contrast to the LDA, the existence of an antiferromagnetic insulating solution for the undoped system makes it possible to study the softening of the half-breathing phonon under doping. We find that although the HF approximation and the t - J model give similar softenings, these softenings happen in quite different ways. We also find that the HF approximation gives an incorrect doping and \mathbf{q} dependence for the softening and too small a width for the (half-)breathing phonon.

I. INTRODUCTION

The electron-phonon coupling for high- T_c cuprates has recently attracted much interest. Lanzara *et al.*¹ discovered strong coupling to a mode at 70 meV in many cuprates. The coupling was ascribed to a half-breathing phonon along the (1,0,0) direction. This is an in-plane bond-stretching mode, where the vibrations are primarily due to two of the four O atoms surrounding a Cu atom in the CuO_2 plane. Lanzara *et al.*¹ deduced a rather strong apparent electron-phonon coupling $\lambda \sim 1$. The half-breathing phonon shows an anomalous softening when the cuprates are doped, in particular towards the zone boundary.^{2,3,4,5} The softening of other phonons upon doping can be explained as a screening of the ions in the doped system.² The softening of the half-breathing mode, however, cannot be described in a shell model with conventional parameters.² This supports the idea that this phonon has substantial electron-phonon coupling, which would lead to a reduction of the frequency in the doped but not in the undoped system. This phonon has an appreciable broadening,³ which can also be explained in terms of a substantial electron-phonon coupling. From the broadening one could estimate an electron phonon coupling for this mode of the order of $\lambda \sim 0.2 - 0.3$, using the formula of Allen⁶ and the density of states of Mattheiss.⁷ Anomalous behavior of bond-stretching modes has also been observed in other compounds.^{8,9,10}

The half-breathing phonon has been studied^{11,12,13,14} within the t - J model,¹⁵ and a substantial softening was found.^{11,12,14} Phonons and the electron-phonon interaction have also been studied^{16,17,18} extensively within the local-density approximation (LDA).¹⁹ Bohnen *et al.*¹⁸ found phonon frequencies in good agreement with experiment for $\text{YBa}_2\text{Cu}_3\text{O}_7$. In particular, the frequency of the half-breathing mode along the (1,0,0) direction was found to be anomalously soft, in agreement with experiment. Since LDA does not describe antiferromagnetism in the undoped system, however, it cannot properly describe phonons in the undoped case. It is therefore

not clear how much the phonon is softened under doping in the LDA. Furthermore, LDA calculations show a weak electron-phonon coupling to the half-breathing phonon, with λ at the zone boundary being ~ 0.01 .¹⁸ This is in disagreement with the large width of the half-breathing phonon, which is believed to be due to a rather strong electron-phonon coupling. The weak coupling raises questions about the reason for the low frequency of the half-breathing phonon in the LDA calculation for the doped system.

To address these issues, we here study the three-band model,²⁰ including a Cu $d_{x^2-y^2}$ and two O p -orbitals per unit cell. We allow displacements of the atoms from their equilibrium positions and take the corresponding changes of hopping integrals into account. In this model we can study phonons. We solve the model using a Hartree-Fock (HF) mean-field approximation, which may be expected to simulate features of the LDA for the doped system. For instance, we find a similar width for the half-breathing phonon as in the LDA. In contrast to LDA, however, this approximation gives an antiferromagnetic solution for the undoped system. We can therefore obtain the softening upon doping within this framework. The softening of the half-breathing phonon is indeed found to be of the same order of magnitude as the experimental result, supporting the idea that the LDA can describe the softening.

Alternatively, a t - J model with phonons can be derived from the three-band model. This model is solved using exact diagonalization.¹⁴ Thereby, many-body effects are included, and the interplay between electron-phonon and electron-electron interactions are considered in a more explicit way. In this paper we compare the results in these two approaches.

We find that the HF solution of the three-band model and the t - J model give a comparable softening of the half-breathing phonon. This happens, however, in a very different way in the two approaches. Furthermore, we find that the dependence on doping and on \mathbf{q} is rather different in the two approaches. In the t - J model, the softening is $\sim \delta$ for small δ , while the doping dependence

is weaker in the HF solution. The t - J model gives a smaller softening for the $\mathbf{q} = (1, 1)\pi/a$ breathing mode than for the $\mathbf{q} = (1, 0)\pi/a$ half-breathing mode, while the opposite is found in the HF approximation. In both cases t - J results are in better agreement with experiment.

In Sec. II we introduce the models and in Sec. III the methods. The results are presented in Sec. IV. The results of the HF approximation for the three-band model are compared with the exact diagonalization results of the t - J model in Sec. V.

II. MODELS

We study the three-band model with N unit cells

$$H = \varepsilon_d \sum_{i\sigma} n_{id\sigma} + \varepsilon_p \sum_{j\sigma} n_{jp\sigma} + U \sum_i n_{id\uparrow} n_{id\downarrow} \quad (1)$$

$$+ \sum_{\langle i,j \rangle \sigma} [t_{ij}^{pd} \psi_{id\sigma}^\dagger \psi_{jp\sigma} + h.c.] + \sum_{\langle i,j \rangle \sigma} t_{ij}^{pp} \psi_{ip\sigma}^\dagger \psi_{jp\sigma},$$

where $n_{id\sigma}$ and $n_{jp\sigma}$ are the occupation numbers for the N $3d$ -orbitals and the $2N$ $2p$ -orbitals, respectively, and $\psi_{id\sigma}$ and $\psi_{jp\sigma}$ are the corresponding annihilation operators. The site energies are ε_d and ε_p . There is a Coulomb integral U , acting between two $3d$ -electrons on the same Cu site. The model includes hopping between nearest neighbor Cu and O atoms and between the O atoms which are nearest neighbors of a particular Cu atom.²¹ These hopping integrals are given by t^{pd} and t^{pp} , respectively, with the signs determined by the relative orientations of the orbitals involved. Displacing an atom leads to changes of both electrostatic potentials and hopping integrals. Electrostatic potentials are screened differently in the doped and undoped systems. It was found, however, that the change of screening does not strongly influence the half-breathing phonon.³ We therefore assume here that the changes of hopping integrals are the dominating effects.²²

We assume the hopping integral t^{pd} has a power dependence on the atomic separation d , i.e.,

$$t^{pd}(d) = \left(\frac{a/2}{d}\right)^{3.5} t^{pd0} \quad (2)$$

where a is the lattice parameter. The exponent 3.5 for t^{pd} was estimated from LDA band structure calculations.²³ We neglect the phonon modulation of t_{pp} .

This model can be solved directly as it stands within some approximation, here the Hartree-Fock approximation. We can, however, also derive a t - J model with phonons, and then solve this model. The t - J model has one site per Cu atom. In the undoped system, there is one hole per site. Doping introduces additional holes, which primarily sit on O sites. These O holes form Zhang-Rice singlets with neighboring Cu holes.¹⁵ It is then assumed that each site is occupied by either a d -hole or a Zhang-Rice singlet. Expressing the atomic displacements in terms of phonon operators and working to linear

order in the displacements leads to the t - J model with phonons¹⁴

$$H_{t-J} = J \sum_{\langle i,j \rangle} \left(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{n_i n_j}{4} \right) - t \sum_{\langle i,j \rangle \sigma} \tilde{c}_{i\sigma}^\dagger \tilde{c}_{j\sigma} \quad (3)$$

$$+ \sum_{\mathbf{q}\nu} \omega_\nu(\mathbf{q}) \left(b_{\mathbf{q}\nu}^\dagger b_{\mathbf{q}\nu} + \frac{1}{2} \right)$$

$$+ \sum_{ij\sigma} \tilde{c}_{i\sigma}^\dagger \tilde{c}_{j\sigma} \sum_{\mathbf{q}\nu} g_{ij}^{t-J}(\mathbf{q}, \nu) (b_{\mathbf{q}\nu} + b_{-\mathbf{q}\nu}^\dagger).$$

Here $\tilde{c}_{i\sigma}^\dagger$ creates a d -hole on site i if this site previously had no hole, i.e., if it had a Zhang-Rice singlet. The operator $b_{\mathbf{q},\nu}^\dagger$ creates a phonon with wave vector \mathbf{q} , index ν and frequency $\omega_\nu(\mathbf{q})$. $\delta_{i,j-\hat{x}} = 1$ if site j is one site to the right of i in the x -direction. The formulas for $g_{ij}^{t-J}(\mathbf{q}, \nu)$ have been given elsewhere.¹⁴ While we treat the three-band model in the electron picture, we treat the t - J model in the hole picture.

In deriving this model, we assumed that $t_{pd} \ll |\varepsilon_d - \varepsilon_p|$, U . This is a rather poor approximation for realistic parameters. Here we have somewhat artificially reduced the value of t^{pd0} to 1.2 eV, which gives a realistic²⁴ value of $t = -0.47$ eV if perturbation theory is used, and probably also more realistic values for g_{ij}^{t-J} , by compensating for some of the effects of perturbation theory.¹⁴ The treatment above neglected quadratic terms, although these also can give a doping dependent contribution to the phonon softening.

III. METHODS

We use a frozen phonon method to calculate the phonon frequency in the HF approximation for the three-band model. This gives the effective Hamiltonian

$$H_{\text{eff}} = \sum_{i\sigma} (\varepsilon_d + U \langle n_{id-\sigma} \rangle) n_{id\sigma} + \varepsilon_p \sum_{j\sigma} n_{jp\sigma} \quad (4)$$

$$- U \sum_i \langle n_{id\uparrow} \rangle \langle n_{id\downarrow} \rangle$$

$$+ \sum_{\langle i,j \rangle \sigma} [t_{ij}^{pd} \psi_{id\sigma}^\dagger \psi_{jp\sigma} + h.c.] + \sum_{\langle i,j \rangle \sigma} t_{ij}^{pp} \psi_{ip\sigma}^\dagger \psi_{jp\sigma},$$

where $\langle n_{id-\sigma} \rangle$ is the expectation value of $n_{id-\sigma}$. We also introduce the effective level

$$\varepsilon_{d\sigma}^{\text{eff}} = \varepsilon_d + U \langle n_{id-\sigma} \rangle. \quad (5)$$

A static distortion is built into the lattice and the change of the total energy is calculated. From this the interaction with the electrons can be deduced and the softening of the phonon obtained. The displacements of the atoms in the lattice is denoted by $\{u\}$. The energy of the electronic system is then

$$E[\{u\}] = \text{Tr}(H[\{u\}]\rho[\{u\}]), \quad (6)$$

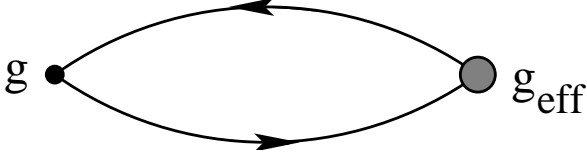


FIG. 1: Diagram describing the linear response. $g \sim \partial H / \partial u$ and $g_{\text{eff}} \sim \partial H_{\text{eff}} / \partial u$ describe the bare and screened perturbations due to a phonon.

where $\rho[\{u\}]$ is the density matrix, obtained in some approximation, e.g. the HF approximation. Using the Hellmann-Feynman theorem, it follows that

$$\frac{\partial^2 E}{\partial u^2} = \text{Tr} \left(\frac{\partial H}{\partial u} \frac{\partial \rho}{\partial u} \right) + \text{Tr} \left(\frac{\partial^2 H}{\partial u^2} \rho \right) \equiv \frac{\partial^2 E^{(1)}}{\partial u^2} + \frac{\partial^2 E^{(2)}}{\partial u^2}. \quad (7)$$

From the total energy calculation, we can deduce both $\partial^2 E / \partial u^2$ and $(\partial^2 E / \partial u^2)^{(i)}$, $i=1, 2$. $(\partial^2 E / \partial u^2)^{(1)}$ describes how a first order change in the external Hamiltonian leads to a first order change in the density matrix, which acts back at the Hamiltonian. This contribution can be calculated in linear response

$$\frac{\partial \rho}{\partial u} = \chi \frac{\partial H_{\text{eff}}}{\partial u}, \quad (8)$$

where χ is the response function for noninteracting electrons and the derivative of the effective Hamiltonian is obtained from the total energy calculation. Thus we have

$$\frac{\partial^2 E^{(1)}}{\partial u^2} \equiv \text{Tr} \left(\frac{\partial H}{\partial u} \frac{\partial \rho}{\partial u} \right) = \text{Tr} \left(\frac{\partial H}{\partial u} \chi \frac{\partial H_{\text{eff}}}{\partial u} \right). \quad (9)$$

We introduce a dielectric function

$$\epsilon = \text{Tr} \left(\frac{\partial H}{\partial u} \chi \frac{\partial H}{\partial u} \right) / \text{Tr} \left(\frac{\partial H}{\partial u} \chi \frac{\partial H_{\text{eff}}}{\partial u} \right). \quad (10)$$

The result in Eq. (9) can also be obtained from a diagrammatic technique. It is described by a bubble diagram, as shown in Fig. 1. This is the only diagram which enters in the HF approximation. We observe that the screening of the perturbation, described by g_{eff} , enters at one of the vertices. Using g_{eff} at both vertices would lead to double counting. By using the diagrammatic approach, we can obtain not only a contribution to the energy but also the width of the phonon.

IV. RESULTS

Below we present results for the three-band model in the Hartree-Fock approximation, using the parameters $t^{pd0} = 1.6$ eV, $t^{pp} = 0$ and $U = 8$ eV. The lattice parameter is $a = 3.8$ Å. We have adjusted ϵ_p so that the separation between the effective $3d$ -level and $2p$ -levels

$$\epsilon_d^{\text{eff}} - \epsilon_p^{\text{eff}} \equiv \epsilon_d + U \langle n_{d\sigma} \rangle - \epsilon_p = 3 \text{ eV}, \quad (11)$$

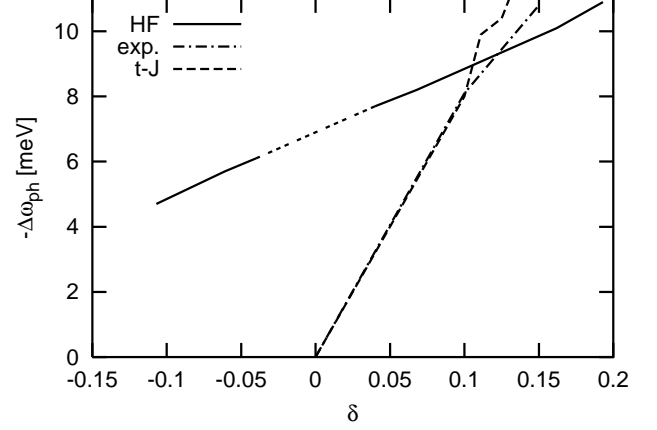


FIG. 2: Softening $\Delta\omega_{ph}$ for the zone boundary half-breathing phonon. Results are given in the HF approximation (full line), the t - J model (dashed line) and according to experiment (dash-dotted line) as a function of the hole doping δ . The lines serve as a guide for the eye between the few points in the t - J model and according to experiment. The HF approximation refers to results for the shift in a paramagnetic calculation for doping δ relative to an antiferromagnetic calculation for $\delta = 0$. The dashed part of the HF line indicates schematically that the systems goes antiferromagnetic for small dopings.

where $\langle n_{d\sigma} \rangle$ is the average occupation of the $3d$ -levels per spin. This is a typical LDA estimate for $\epsilon_d^{\text{eff}} - \epsilon_p^{\text{eff}}$ in a three-band model.²¹ We perform two calculations, one for the undistorted lattice and one for a lattice where a phonon has been built in. This gives the second derivative, $\partial^2 E / \partial u^2$. From this derivative we obtain the softening of the phonon due to the interaction with the electrons in the model, reducing the frequency ω_{ph0} to ω_{ph} . Here ω_{ph0} is assumed to be due to forces not included in the model in Eq. (1), e.g., electrostatic forces and core-core overlap effects. The calculations were performed for a cluster of 32×32 CuO_2 units and periodic boundary conditions. The doping was chosen in such a way that degenerate levels were either completely full or completely empty, i.e., all “shells” were either full or empty.

We first consider the half-breathing phonon for $\mathbf{q} = (1, 0)\pi/a$, where the two O atoms at $(a/2, 0)$ and $(-a/2, 0)$ move towards (or away from) from the Cu atom at $(0, 0)$. We perform a calculation for the undoped system, having five electrons per unit cell, and allowing for spin-polarization. We adjust ω_{ph0} so that the softened frequency ω_{ph} is 0.080 eV for the zone boundary half-breathing phonon, as is found experimentally.

The result as a function of the hole doping δ ($\delta < 0$ means electron doping) is shown in Fig. 2. The doping dependence is relatively weak. Since the undoped system is antiferromagnetic but the doped system is (assumed to be) paramagnetic, as found experimentally, the softening is not necessarily small for small dopings. The spin-polarized system has a large gap of about 4.6 eV. Due to this gap, the response of the system to a phonon

is substantially weaker than for the paramagnetic state. For instance, $[\partial^2 E / \partial u^2]^{(1)}$ contributes a softening of only about 4 meV for the spin-polarized system but 6 meV for a non spin-polarized system with a similar number of electrons. Similarly, the contributions of $[\partial^2 E / \partial u^2]^{(2)}$ are about 8 and 13 meV, respectively.

We find that screening reduces the quantity $[\partial^2 E / \partial u^2]^{(1)}$ by about a factor of two, i.e., $\epsilon \approx 2$ in Eq. (10). By evaluating the diagram in Fig. 1, we find that the zone boundary half-breathing phonon is broadened by about 0.4 meV for $\delta = 0.16$. This is similar to what Bohnen *et al.*¹⁸ found in an LDA calculation.

It is interesting to compare the half-breathing phonon and the $\mathbf{q} = (1, 1)\pi/a$ breathing phonon. In the latter case all four O atoms surrounding a Cu atom move towards this atom. In the model considered above ($t^{pp} = 0$) and for $\delta = 0$, the model has nesting for $\mathbf{q} = (1, 1)\pi/a$. The result would be a very strong response for small δ , making the calculation rather meaningless. Instead we consider $t^{pp} = 1.1$ eV.²¹ This changes the Fermi surface and avoids an unrealistically strong nesting. In this case we adjust ω_{ph0} so that $\omega_{ph} = 0.090$ eV in the spin-polarized calculation for the undoped system, as found experimentally. For the doping $\delta = 0.096$ we find that the $\mathbf{q} = (1, 1)\pi/a$ breathing phonon is softened by 11 meV. This is a larger softening than was found in Fig. 2 for this doping. We have also performed a calculation for the $\mathbf{q} = (1, 0)\pi/a$ half-breathing phonon in this model and for this doping. The softening is 7 meV, which again is smaller than for the breathing phonon. This is contrary to experiment, where a larger softening is found for the half-breathing phonon.

V. COMPARISON OF THE t - J MODEL AND HF SOLUTION OF THE THREE-BAND MODEL

To make contact with the t - J model, we transform the three-band model to a one-band model. We assume that the O $2p$ -levels are far below the Cu $3d$ -levels (in the electron picture). We can then project out the O $2p$ -levels and obtain a model with just effective Cu $3d$ -levels. This model can be compared with the t - J model, since both models have one band. Here we focus on the linear response term $(\partial^2 E / \partial u^2)^{(1)}$ in Eq. (9), which are of the same order of magnitude in the t - J model and the HF approximation for a typical $\delta \sim 0.1$.

We introduce a projection operator P , which projects out the Cu $3d$ -levels, and its complement $Q = 1 - P$. Considering the resolvent operator of the HF Hamiltonian, we obtain

$$P(z - H)^{-1}P \quad (12)$$

$$= [P(z - H)P - PHQ(z - QHQ)^{-1}QPH]^{-1},$$

where z is some typical energy. We then obtain the ef-

fective one-band parameters

$$\epsilon_{id\sigma}^{\text{One}} = \epsilon_d + \sum_{\langle j \rangle} \frac{(t_{ij}^{pd})^2}{z - \epsilon_p},$$

$$t_{ii'}^{\text{One}} = \frac{t_{ij}^{pd} t_{ji'}^{pd}}{z - \epsilon_p}, \quad (13)$$

where the sum over j for $\epsilon_{id\sigma}^{\text{One}}$ runs over the nearest O neighbors of Cu and j for $t_{ii'}^{\text{One}}$ refers to the common nearest neighbor O atom of the Cu atoms i and i' . We first consider the unperturbed (no phonon) system. We choose z to be in the middle of the band and solve the self-consistent equations

$$\epsilon_d^{\text{One}} = \epsilon_d + \frac{4(t^{pd})^2}{\epsilon_d^{\text{One}} - \epsilon_p} \quad (14)$$

$$t_{ii'}^{\text{One}} = -\frac{(t^{pd})^2}{\epsilon_d^{\text{One}} - \epsilon_p},$$

where the factor 4 for ϵ_d^{One} comes from the four O neighbors of a Cu atom.

We then introduce a phonon in the system and ask for the linear response of the electronic system. A perturbation term is introduced in the one-band Hamiltonian

$$\partial \epsilon_{id\sigma} = \sum_{\langle j \rangle} 2 \frac{t_{ij}^{pd} \partial t_{ij}^{pd}}{\epsilon_d^{\text{One}} - \epsilon_p}, \quad (15)$$

where ∂t_{ij}^{pd} are the changes in the Cu-O hopping integrals. To linear order there is no change in $t_{ii'}^{\text{One}}$.

For a half-breathing phonon at the zone boundary, the on-site perturbation is

$$\frac{\partial H}{\partial u} u = 4t_{pd} \frac{\partial t_{pd}}{\partial r} \frac{1}{\epsilon_d^{\text{One}} - \epsilon_p} u, \quad (16)$$

where u is the absolute value of the phonon amplitude. The quantity $\partial H / \partial u$ enters in the calculation of $(\partial^2 E / \partial u^2)^{(1)}$ in Eq. (9).

In the t - J model, the on-site perturbation is¹⁴

$$4t_{pd} \frac{\partial t_{pd}}{\partial r} \left(\frac{2\lambda^2 - 1}{|\epsilon_d - \epsilon_p|} + \frac{2\lambda^2}{U - |\epsilon_d - \epsilon_p|} \right) u, \quad (17)$$

where $\lambda = 0.96$. The first term comes from the hopping of a $3d$ -hole into the O $2p$ -states and the second term from the hopping of a O $2p$ -hole into the Cu $3d$ -state. The second term has no correspondence in Eq. (16). Equation (17) has an additional factor 2 coming from a phase coherence factor in the Zhang-Rice singlet. This results from the singlet being explicitly written as a sum of two terms. Both these effects are genuine many-body effects. The -1 in the first term in Eq. (17) results from taking the difference in the energy gain of a Zhang-Rice singlet and a single $3d$ -hole.

TABLE I: Contributions to the phonon softening in the t - J model and in the HF solution of the three-band model. Here $\Delta \equiv |\varepsilon_d^{\text{One}} - \varepsilon_p| = |\varepsilon_d - \varepsilon_p|$.

Source	t - J	HF	Ratio
Coupling	$[(2\lambda^2 - 1)/\Delta + 2\lambda^2/(U - \Delta)]^2$	$(1/\Delta)^2$	≈ 3
Sum rule	$\approx 2\delta\pi N$	$\approx \pi N$	$\approx 2\delta$
Screening	1	≈ 0.5	≈ 2
Denominator		≈ 1	
Product			12 δ

We find that this on-site coupling dominates over the off-site coupling.¹⁴ In the qualitative discussion we therefore only consider the on-site coupling $g_{ii}^{t-J}(\mathbf{q}) \equiv g(\mathbf{q})$. The phonon self-energy in the t - J model is

$$\Pi(\mathbf{q}, \omega) = \frac{g(\mathbf{q})^2 \chi^{t-J}(\mathbf{q}, \omega)}{1 + g(\mathbf{q})^2 \chi^{t-J}(\mathbf{q}, \omega) D_0(\mathbf{q}, \omega)}, \quad (18)$$

where $D_0(\mathbf{q}, \omega)$ is the noninteracting phonon Green's function. We find that the second term in the denominator is small for the parameters considered here. In the formal discussions below we therefore neglect it. The phonon self-energy is then proportional to the response function. This result can then be directly compared with the result in Eq. (9) for the one-band model. In both cases the response function is multiplied by the appropriate coupling constant squared, given by Eq. (16) and Eq. (17), respectively.

To compare the t - J model with the one-band model, we put $|\varepsilon_d^{\text{One}} - \varepsilon_p| = |\varepsilon_d - \varepsilon_p| \equiv \Delta = 3$ eV and $U = 8$ eV.²⁵ We find that the square of Eq. (17) is about a factor of three larger than the square of Eq. (16). This difference due to differences in coupling constants is shown in Table I.

The linear response of the one-band model is given by

$$\chi^{\text{HF}}(\mathbf{q}, \omega) = 2 \sum_{\mathbf{k}} [1 - f(\mathbf{k} + \mathbf{q})] f(\mathbf{k}) \times \left(\frac{1}{\omega - \omega(\mathbf{k}, \mathbf{q}) + i0^+} - \frac{1}{\omega + \omega(\mathbf{k}, \mathbf{q}) - i0^+} \right) \quad (19)$$

where $f(\mathbf{k})$ is the Fermi function for a state with wave vector \mathbf{k} and energy $\varepsilon(\mathbf{k})$ and $\omega(\mathbf{k}, \mathbf{q}) = \varepsilon(\mathbf{k} + \mathbf{q}) - \varepsilon(\mathbf{k})$. We have the sum-rule

$$\frac{1}{N} \sum_{\mathbf{q} \neq 0} \int_{-\infty}^{\infty} |\text{Im} \chi^{\text{HF}}(\mathbf{q}, \omega + i0^+)| = 4\pi n(1 - n)N \approx \pi N, \quad (20)$$

where N is the number of sites and n is the fractional filling of the band. Typically, we are interested in a system with $n = (1 - \delta)/2 \approx 0.5$ electrons per site and spin, which leads to the right hand side of Eq. (20). For the t - J model we ask for the carrier-carrier response function

$$\chi^{t-J}(\mathbf{q}, \omega) = \sum_{\nu} |\langle \nu | \rho(\mathbf{q}) | 0 \rangle|^2 \times \left(\frac{1}{\omega - \omega_{\nu} + i0^+} - \frac{1}{\omega + \omega_{\nu} - i0^+} \right), \quad (21)$$

where $|\nu\rangle$ is an excited many-electron state with the excitation energy ω_{ν} and $\rho(\mathbf{q})$ is carrier density operator. One finds¹²

$$\frac{1}{N} \sum_{\mathbf{q} \neq 0} \int_{-\infty}^{\infty} |\text{Im} \chi^{t-J}(\mathbf{q}, \omega + i0^+)| = 2\pi N \delta(1 - \delta). \quad (22)$$

Eqs. (20) and (22) differ by approximately a factor of 2δ for small δ (see Table I).

The two approaches further differ by the screening in the HF approach, discussed in Eq. (10). This reduces the HF result by roughly a factor of two. Finally, we have to consider that a typical energy denominator in Eq. (20) and Eq. (21) are different. Calculating the average $\langle 1/\omega \rangle$, we find comparable results for the two models. As can be seen from Table I, the difference between the two approaches results in a ratio of about 12 δ . For $\delta \sim 0.1$, the two results are then similar. This indicates why the t - J model and the HF solution of the three-band model can give similar softening of the half-breathing mode although the physics is quite different.

We next consider the imaginary part of the phonon self-energy Π , which gives the phonon width. As an orientation, we first consider a simple model. Since $\text{Im} \chi(\omega) \sim \omega$ for small ω , we assume

$$\text{Im} \Pi(\mathbf{q}, \omega) = \begin{cases} A\omega, & \text{if } |\omega| \leq W; \\ 0, & \text{otherwise,} \end{cases} \quad (23)$$

where A is some constant. From the Kramers-Kronig relation, we can then derive

$$\frac{\gamma}{-\Delta\omega_{ph}} = \pi \frac{\omega_{ph}}{W}, \quad (24)$$

where $\gamma = 2\text{Im} \Pi(\mathbf{q}, \omega)$ is the full width at half maximum of the phonon and $\Delta\omega_{ph}$ is its shift.

Figure 3 compares $\text{Im} \Pi(\mathbf{k}, \omega)$ for the half-breathing phonon in the one- and three-band models and the breathing phonon in the three-band model. The one-band model was constructed to describe what happens close to E_F and therefore the one- and three-band models agree very well for small ω . For $|\omega| \gg 0$, the one-band model gives a larger $|\text{Im} \Pi(\mathbf{q}, \omega)|$ than the three-band model, and $|\text{Re} \Pi(\mathbf{q}, \omega)|$ is overestimated correspondingly in the one-band model. Appropriate numbers for the half-breathing phonon and the one-band model are $W = 2$ eV, $\omega_{ph} = 0.07$ eV, $\Delta\omega_{ph} = -0.007$ eV. Inserting this in Eq. (24) leads to $\gamma = 0.8$ meV. This is about twice the width actually calculated. The reason for this overestimate is that $\text{Im} \Pi(\mathbf{q}, \omega)$ is actually smaller than assumed in Eq. (22) for small ω .

Figure 3 also shows the HF result for the $\mathbf{q} = (1, 1)\pi/a$ breathing phonon. These results were obtained for $t^{pp} = 1.1$ eV. There is then no strong nesting of the Fermi surface. The HF approximation, nevertheless, gives a larger broadening for the $\mathbf{q} = (1, 1)\pi/a$ breathing phonon than for the $\mathbf{q} = (1, 0)\pi/a$ half-breathing phonon, whether the latter is calculated for $t^{pp} = 0$ or $t^{pp} = 1.1$ eV. As is

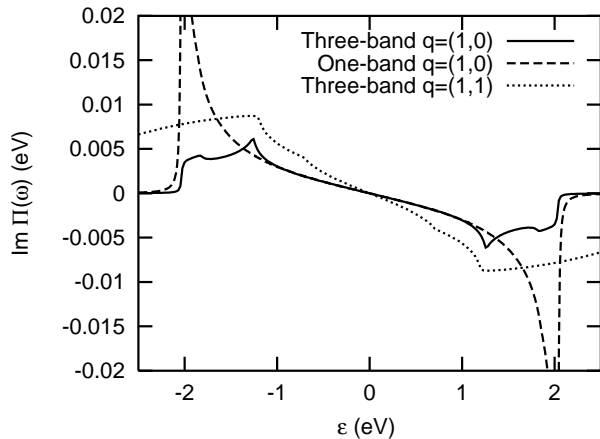


FIG. 3: $\text{Im } \Pi(\mathbf{q}, \omega)$ for the $\mathbf{q} = (1, 0)\pi/a$ half-breathing mode in the three-band model (full line) and the one-band model (dashed line) and for the $\mathbf{q} = (1, 1)\pi/a$ breathing mode (dotted line). The doping is $\delta = 0.1$.

well-known,¹⁶ this is due to the fact that the wave vector $\mathbf{q} = (1, 1)\pi/a$ fits better to the traces of nesting left over for $t^{pp} = 1.1$ eV.

To study the phonon width in the t - J model, we calculate the phonon self-energy.²⁶ We calculate the phonon spectral function $B(\mathbf{q}, \omega)$ using exact diagonalization. A Hilbert transform can then be used to obtain the phonon Green's function $D(\mathbf{q}, \omega)$. The phonon self-energy $\Pi(\mathbf{q}, \omega)$ is calculated by inverting

$$D^{-1}(\mathbf{q}, \omega) = D_0^{-1}(\mathbf{q}, \omega) - \Pi(\mathbf{q}, \omega), \quad (25)$$

where $D_0(\mathbf{q}, \omega)$ is the noninteracting phonon Green's function. This approach has important advantages for small systems. $B(\mathbf{q}, \omega)$ has too few structure to determine the phonon width. A broadened version of $\Pi(\mathbf{q}, \omega)$, however, can give such information.²⁶ Results for $\Pi(\mathbf{q}, \omega)$ are shown in Fig. 4.

In the view of Eq. (24), one might have expected the width of the half-breathing phonon to be similar in the HF approximation and the t - J model, since the shifts are similar. This is not true, however, since the frequency dependence differs strongly from the linear dependence assumed in Eq. (23). This is illustrated in Fig. 4. The figure shows that for the t - J model with $J = 0$, some spectral weight has been moved to small frequencies due to the hopping constraint, which creates low energy excitations. This is even more true for the finite J case ($J/t = 0.3$). The present clusters are too small to give reliable results, in particular for the low-lying excitations, and the results above should be considered as qualitative. They illustrate the general trend, however, of transferring

some spectral weight to small frequencies, which tends to lead to a substantially increased width of the half-breathing phonon.

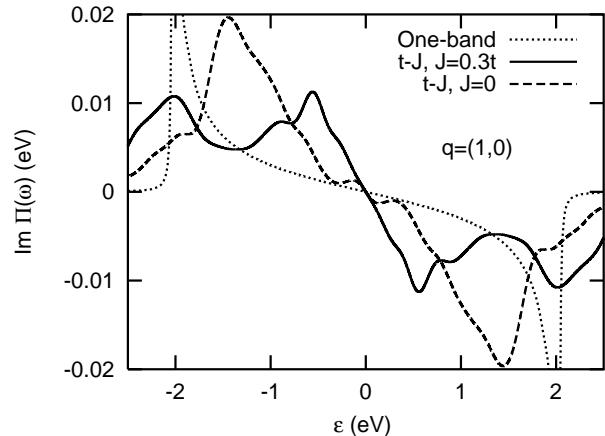


FIG. 4: $\text{Im } \Pi(\mathbf{q}, \omega)$ for the $\mathbf{q} = (1, 0)\pi/a$ half-breathing mode in the t - J model for $J/t = 0.3$ (full line) and $J/t = 0$ (dashed line) and in the one-band model (dotted line). The results for the t - J model were obtained for a 4×4 cluster. The doping is $\delta = 0.125$.

VI. SUMMARY

We have studied the properties of the half-breathing phonon in the three-band model of a high- T_c cuprate. The results in a t - J model with phonons and the HF approximation of the three-band model were compared. Although the two approaches give similar softenings at typical dopings δ , the underlying physics is quite different. The hopping constraint in the t - J model, resulting from the strong Coulomb repulsion, leads to a strong reduction of the response to a phonon. This reduction is, however, partly compensated by several other effects. In particular, the coherent hopping in the formation of the Zhang-Rice singlet tends to increase the coupling in the t - J model. We find that the doping and \mathbf{q} dependences for the (half-)breathing mode are quite different in the two approaches, with the t - J model giving better agreement with experiment. The HF approximation also gives a too small width for the half-breathing phonon. We therefore conclude that many-body effects play an important role for the interactions of the half-breathing phonon with the electrons.

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